

SUPPLEMENTARY DATA

Conformational stability and activity analysis of two hydroxymethylbilane synthase mutants, K132N and V215E, with different phenotypic association with acute intermittent porphyria

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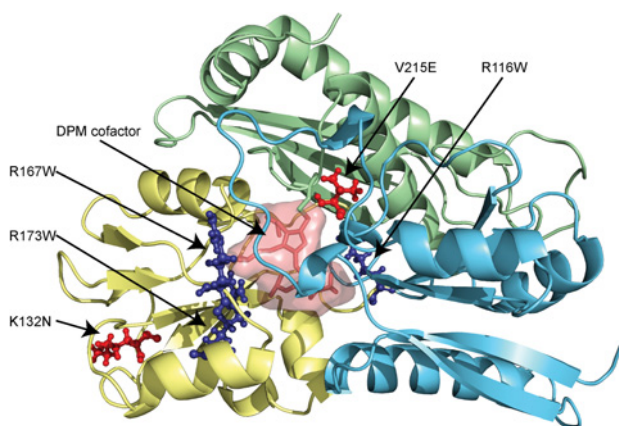


Figure S1 Structural model of HMBS

The location of the two novel mutations studied in this work, K132N and V215E, are presented as ball-and-sticks in red, whereas the three previously reported mutations (R116W, R167W and R173W) are presented as ball-and-sticks in dark blue. The complete structural model of HMBS was constructed with Modeller [1] based on multiple templates (PDB IDs: 1AH5, 1PDA, 1GTK, 1YPN, 3ECR and 3EQ1). Coordinates for residues 55–75 have been issued to loop optimization constructing a large set of possible confirmations. The lowest energy structure was chosen, and further refined with energy minimization using Amber 10 [2].

REFERENCES

- 1 Fiser, A. and Sali, A. (2003) Modeller: generation and refinement of homology-based protein structure models. *Methods Enzymol.* **374**, 461–491
- 2 Case, D. A., Cheatham, 3rd, T. E., Darden, T., Gohlke, H., Luo, R., Merz, Jr, K. M., Onufriev, A., Simmerling, C., Wang, B. and Woods, R. J. (2005) The Amber biomolecular simulation programs. *J. Comput. Chem.* **26**, 1668–1688

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